

allyl 1-propenyl disulfide

Inchi: InChI=1S/C6H10S2/c1-3-5-7-8-6-4-2/h3-4,6H,1,5H2,2H3/b6-4+
InchiKey: KBXOGESWPIVMNJ-GQCTYLIASA-N
Formula: C6H10S2
SMILES: C=CCSSC=CC
Mol. weight [g/mol]: 146.27

Physical Properties

Property code	Value	Unit	Source
gf	233.94	kJ/mol	Joback Method
hf	159.22	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.087		Crippen Method
mvol	119.500	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1080.00		NIST Webbook
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tb	475.08	K	Joback Method
tc	703.14	K	Joback Method
tf	219.34	K	Joback Method
vc	0.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.99	J/mol×K	475.08	Joback Method
cpg	230.97	J/mol×K	513.09	Joback Method
cpg	241.30	J/mol×K	551.10	Joback Method
cpg	251.02	J/mol×K	589.11	Joback Method
cpg	260.14	J/mol×K	627.12	Joback Method
cpg	268.70	J/mol×K	665.13	Joback Method
cpg	276.70	J/mol×K	703.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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